J. Mod. Transport. (2014) 22(3):183–186
DOI 10.1007/s40534-014-0045-z

www.springer.com/40534

The electronic structure of Nb_3Al/Nb_3Sn, a new test case for flat/steep band model of superconductivity

Yanlong Ding · Shuiquan Deng · Yong Zhao

Received: 3 December 2013 / Revised: 12 February 2014 / Accepted: 15 March 2014 / Published online: 2 April 2014

Abstract In this work, we choose Nb_3Al/Nb_3Sn as a new test case for flat/steep band model of superconductivity. Based on the density functional theory in the generalized gradient approximation, the electronic structure of Nb_3Al/Nb_3Sn has been studied. The obtained results agree well with those of the earlier studies and show clearly flat bands around the Fermi level. The steep bands as characterized in this work locate around the M point in the first Brillouin zone. The obtained results reveal that Nb_3Al/Nb_3Sn fits more to the "Flat/steep" band model than to the van-Hove singularity scenario. The flat/steep band condition for superconductivity implies a different thermodynamic behavior of superconductors other than that predicted from the conventional BCS theory. This observation sets up an indicator for selecting a suitable superconductor when its large-scale industrial use is needed, for example, in superconducting maglev system or ITER project.

Keywords Nb_3Al/Nb_3Sn · Electronic structure · Flat/steep band model · First-principle

1 Introduction

Superconductors have found widespread applications ranging from civil to military uses. The superconductor-based Magnetic Resonance Imaging (MRI) technique used in many hospitals, the superconducting super-collider project in Texas USA, the Large Hadron Collider (LHC) in CERN, the ITER project, the Experimental Advanced Superconducting Tokomak (EAST) in China and so on are all examples where superconductors are necessary materials. Another important application is the superconducting magnetic levitation system, which not only saves much of the electrical energy but also saves the space and weight of the vehicle and dramatically increases its speed [1]. Such important applications require deeper and exact understanding of the properties, e.g. mechanical and critical ones, of a superconductor.

The flat/steep band model [2, 3] for superconductivity has been proposed over many years in attempting to understand superconductivity from a chemistry point of view. The previous studies [4] indicate that the electronic structures of conventional elemental and complex superconductors show good agreement with this model. However, this model met a non-trivial challenge in the case of Calcium, although it finally proved to be the shortcoming of the first-principle methods instead of that of the flat/steep band model [5]. Nb_3Al/Nb_3Sn is a typical A15 superconductor, which though has been intensively studied, respectively, remains a challenge to the existing theories regarding their strain and scale-dependent critical properties such as the upper critical magnetic field and current density. On the other hand, Nb_3Al and Nb_3Sn have very important applications on the thermonuclear fusion experimental reactor as magnetic plasma-control materials for their overall merit factors. The results of earlier studies on the preparations, crystal structures, electronic structures, and various properties of A15 compounds have been systematically reviewed by many authors [6–9]. With respect to the electronic structures of A15 compounds, the earlier studies based on the first-principle methods [10–12] have revealed very flat bands around the Fermi level, which

Y. Ding · S. Deng (✉) · Y. Zhao
Key Laboratory of Magnetic Levitation Technologies and Maglev Trains, Ministry of Education of China, and Superconductivity and New Energy R&D Center, Southwest Jiaotong University, Chengdu 610031, China
e-mail: s.deng@swjtu.edu.cn

implies a van-Hove singularity in A15 system. However, the earlier experimental studies have never observed any Peierls-like structural instability in a wide temperature range. This fact itself indicates that either the flat band feature is over estimated as in the case of Calcium [5] or there are some other factors which counteract the effect of the "flat/bands" or both reasons may play a role. In this work, we study the electronic structure of Nb_3Al/Nb_3Sn using the state-of-the-art first-principle method.

2 Computational details

The electronic structure of Nb_3Al/Nb_3Sn has been calculated using the DFT theory as implemented in the Vienna ab initio simulation package (VASP) [13, 14]. The exchange–correlation potential has been calculated at the generalized gradient approximation (gga) level using the Perdew, Burke and Ernzerhof (PBE) formalism [15]. The $10 \times 10 \times 10$ and $20 \times 20 \times 20$ Monkhorst grids have been used to sample the first BZ for structural relaxation and self-consistent calculations, respectively. The cutoff energy for the plane wave expansion is chosen as 320 eV.

3 Results and discussion

3.1 Crystal structure

Nb_3Al/Nb_3Sn is a typical A15 compound with a space group $Pm\bar{3}n$. The unit cell structure of the compound is shown in Fig. 1. The structure belongs to a simple cubic crystal system and contains six Nb atoms and 2 Al or Sn atoms in one conventional crystallographic unit cell. Each unit cell contains six A-type atoms which lie on the surface of the unit cell and form chains along the axis directions, respectively. On each chain, the A-type atoms distribute equidistantly. The two B-type atoms occupy the corners and the center of a unit cell. The A-type and B-type atoms occupy the 6c and 2a Wyckoff positions of the space group, respectively.

3.2 Electronic structure

The electronic density of states (DOS) of Nb_3Al and Nb_3Sn is shown in Fig. 2. As can be seen from Fig. 2, except for tiny shifts and changes of the peak positions and heights, the overall agreement of the DOS curves of Nb_3Al and Nb_3Sn is very good. The DOS around the Fermi level has a sharp peak, which implies a dramatic change of physical properties if the Fermi level is changed by whatsoever means, e.g. doping or stress. By decomposing the

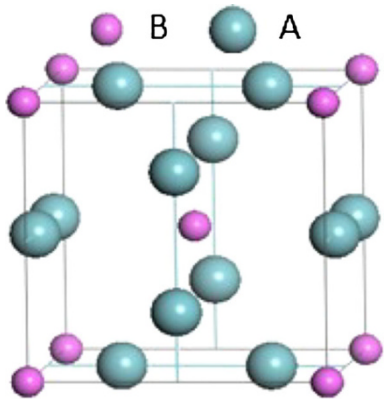

Fig. 1 The crystal structure of an A15 compound

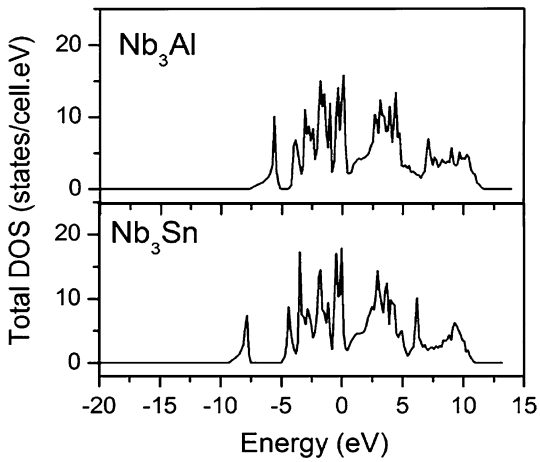

Fig. 2 Density of states of Nb_3Al and Nb_3Sn

electronic states into atomic centered states, we have found that the states around the Fermi level are essentially contributed by the Nb d-states. It is thus obvious that the superconducting properties are crucially decided by the Nb atoms. The energetically lowest peaks at −5.6 and −7.9 eV for Nb_3Al and Nb_3Sn, respectively, are due to the s-states of the B-type atoms. These results agree generally with those of the earlier studies [12, 16].

The first BZ for Nb_3Al and Nb_3Sn is shown in Fig. 3 where the symmetry lines and points are indicated. The coordinates of the symmetry points are (0, 0, 0), (1, 0, 0), (1, 1, 0), (1, 1, 1), for Γ, X, M, and R, respectively. The calculated band structures for Nb_3Al and Nb_3Sn are shown in Figs. 4 and 5, respectively. As for the DOS curves, the band structures of Nb_3Al and Nb_3Sn are quite similar. In both cases, the lowest bands are from the s, p states of the B-type atoms. The bands lying in the range of −3.2 to 5 eV for Nb_3Sn and those between −3 and 4.5 eV for Nb_3Al are contributed by the d-states of Nb. These bands split into the bonding and anti-bonding groups. As shown in Figs. 4 and

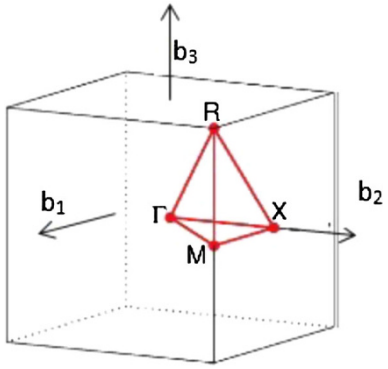

Fig. 3 The first BZ for Nb_3Al and Nb_3Sn structures

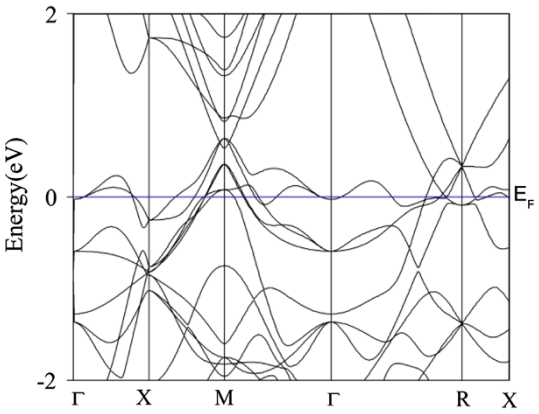

Fig. 4 Electronic band structure of Nb_3Al along symmetry directions

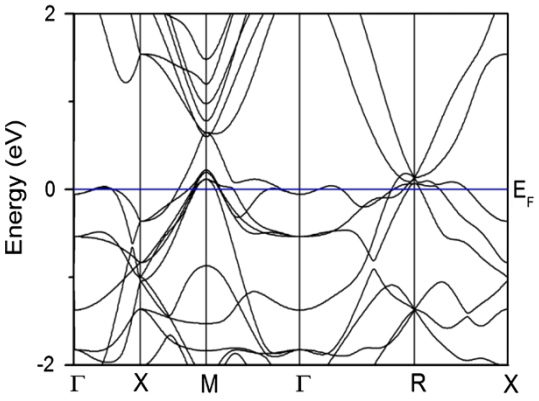

Fig. 5 Electronic band structure of Nb_3Sn along symmetry directions

5, the bonding bands are flatter than the anti-bonding bands.

As revealed in earlier studies [10–12], the bands around the Fermi level of Nb_3Al and Nb_3Sn appear rather flat which is, however, someway an artificial fact due to the chosen large energy scale in representing the band structure. Moreover, the earlier results are not consistent with each other with respect to the accurate position of the flat bands relative to the Fermi level [10–12]. Our investigations on the bands around the Fermi level indicate that the energy bands nearby Γ and R points are significantly flatter than some other bands, while those around the M point are obviously steeper. These steep bands play an important role in counteracting the possible structural instability caused by the high DOS (E_F). In this sense, Nb_3Al and Nb_3Sn fit more to the "flat/steep" band model than to the van-Hove singularity scenario. It is evident that more quantitative experimental data are needed to judge the theoretical results. In particular, the metric details of the Fermi surface are necessary to draw a solid conclusion.

4 Ending remarks

Our studies indicate that the importance of the steep band was not realized in earlier work. The steep band character in the A15 system was neglected due to the use of large energy scale. Our studies indicate clearly that the steep bands locate around the M point in the first BZ (Fig. 4). The obtained results reveal that Nb_3Al/Nb_3Sn fits more to the "flat/steep" band model than to the van-Hove scenario.

Acknowledgements This work is financially supported by the Science Foundation for International Cooperation of Sichuan Province (2014HH0016), the Fundamental Research Funds for the Central Universities (SWJTU2014: A0920502051113-10000), National Magnetic Confinement Fusion Science Program (2011GB112001).

References

1. See for example: http://www.superconductors.org/uses.htm
2. Deng S, Simon A, Köhier J (1998) Supercon-ductivity and chemical bonding in mercury. Angew Chem Int Ed 37(5):640–642
3. Deng S, Simon A, Köhier J (2005) Pairing mechanisms viewed from physics and chemistry. Struct Bond 114:103–141
4. Deng S, Simon A, Köhier J (2008) Calcium d states: chemical bonding of CaC6. Angew Chem Int Ed 47:6703–6706
5. Deng S, Simon A, Köhier J (2002) Flat-band steep band scenario and superconductivity the case of calcium. Solid State Sci 2(1):31–38
6. Weger M, Goldberg B (1973) Lattice and Electronic Properties of the β-Tungstens. Solid State Phys 28:1–177
7. Dew-Hughes D (1975) A-15 compounds: a review. Cryogenics 15(8):435–454
8. Godeke A (2006) A general scaling relation for the critical current density in Nb_3Sn. Supercond Sci Technol 19(10):100–116
9. Glowacki BA (1999) Niobium aluminide as a source of high-current superconductors. Intermetallics 7:117–140
10. Mattheiss LF, Weber W (1982) Electronic structure of cubic V_3Si and Nb_3Sn. Phys Rev B 25(4):2248–2269

11. Klein BM, Boyer LL, Papacon-stantopoulos DA (1978) Self-consistent augmented- plane-wave electronic-structure calculations for the A15 compounds V_3X and Nb_3X, X = Al, Ga, Si, Ge, and Sn. Phys Rev B 18(12):6411–64338
12. Pickett WE, Ho KM, Cohen LM (1979) Electronic properties of Nb3Ge and Nb3Al from self-consistent pseudotential. Phys Rev B 19(4):1734–1750
13. Kresse G, Furthmüller J (1996) Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set. Phys Rev B 54(16):11169–11186
14. Kresse G, Furthmüller J (1996) Efficiency of abinitio total energy calculations for metals and semiconductors using a plane-wave basis set. Comput Mater Sci 6(1):15–50
15. Perdew JP, Burke K, Ernzerhof M (1996) Generalized gradient approximation made simple. Phys Rev Lett 77(3):865–3868
16. Paduani C (2007) Electronic Structure of the A_3B Compounds: A = Nb: B = Al, Ga, Ge, Sn and In. Braz J Phys 37(3B):1073–1079